A Nonlinear, Fully Coupled Adaptive Grid Strategy

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In the numerical simulation of complex physical phenomena, the crucial requirement is predictability, i.e., that the simulation results remain faithful to the actual physical processes. Accordingly, the generation and accumulation of numerical error during the simulation is of special concern, since it introduces distortions that fundamentally alter the fidelity of the simulation. Errors resulting from a lack of spatial resolution are particularly deleterious. However, over-resolving is computationally expensive.

Adaptive grids attempt to provide sufficient resolution where needed while minimizing the computational cost of the simulation. Our emphasis is on moving grid methods (also known as *r*-refinement), where grid points are able to move to follow the solution. The grid positions are determined from a suitable grid evolution equation. While many grid evolution equations have been proposed in the literature [1], here we focus on harmonic maps [2], which are desirable because, under certain conditions, they guarantee the existence and uniqueness of the grid mapping.

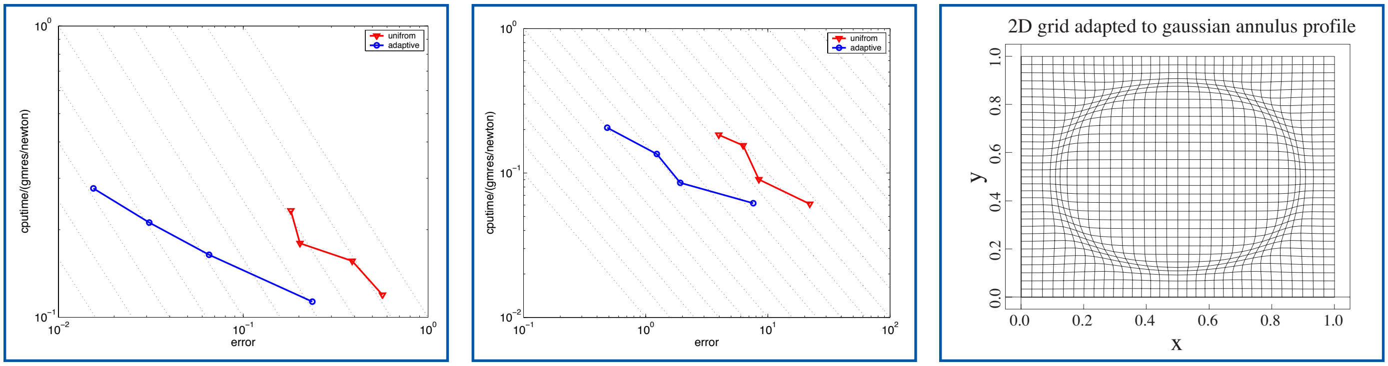
One drawback of harmonic function theory is that the resulting grid evolution equation is generally very nonlinear and stiff. Furthermore, physics models for which spatial adaptation is necessary are typically very stiff as well. For such systems, implicit temporal schemes are preferred for efficiency, as they allow one to use time steps comparable to the dynamical time scale of interest in the problem at hand. However, when coupled to a grid evolution equation, such large implicit time steps may not be advantageous from an accuracy standpoint unless both grid and physics equations are solved in a coupled manner.

The coupled nonlinear solution of such physics-grid systems represents, however, a formidable numerical challenge. It is this challenge that we undertake in this research. At the heart of the matter is to demonstrate that developing a scalable, efficient nonlinear algorithm to solve such systems is indeed possible. We base our strategy on Newton-Krylov methods [3], which are ideally suited for this task owing to their robustness and the possibility of preconditioning.

We proceed to demonstrate two crucial issues. First, that a fully implicit, coupled solution of the grid equation is indeed cost effective with respect to uniform grid computations. And second, that a suitable effective preconditioning strategy based on multigrid (MG) methods for the grid equation in multidimensional problems has been successfully developed.

To determine the cost effectiveness of implicit adaptive grid techniques, we define the *efficacy* η as $\eta = (\text{error} \times \text{cost})^{-1}$. The efficacy is maximized for small errors and small computational costs, making it a suitable figure-of-merit to compare adaptive vs static grid computations. We have performed such a comparison in 1D for two sets of problems: a nonlinear heat equation problem (Marshak wave) and Burgers equation. To generate the adaptive grid we used Winslow's variable diffusion method [1] with an arc-length merit function. In future work we plan to replace the arc-length merit function with more rigorous error estimators [4, 5]. We have employed *unpreconditioned* GMRES as the linear Krylov solver, implemented Jacobian-free [3]. In the comparison, the error is computed with respect to a very fine uniform-grid solution, and the CPU cost is normalized to the number of GMRES iterations to factor out the lack of preconditioning [effective preconditioning results in a constant number of GMRES iterations with grid refinement (see Table 1 for 2D)]. Results are presented in Fig. 1. The adaptive grid outperforms the uniform grid in every respect: for a given cost, the adaptive grid is more accurate, and for a given accuracy, the adaptive grid is cheaper.

While the 1D examples above do not require preconditioning (GMRES gives the exact answer in as many iterations as nodes are present in the grid), scalability



in 2D applications requires effective preconditioning for efficiency. Multigrid methods are ideally suited for this task, as they have been shown in many applications [6, 7] to deliver mesh-independent GMRES convergence rates. For a scalar error monitor function w($\vec{x}$, t), harmonic function theory results in Winslow's variable diffusion method grid evolution equation for $\vec{\xi}(\vec{x}), \nabla \cdot \left(\frac{1}{w} \nabla \xi \right) = 0$, with $\vec{\xi}$ the logical variable and $\vec{x}$ spanning the configuration space. The inverse of this equation [to determine $\vec{x}$ ($\vec{\xi}$)] can be readily expressed in terms of the contravariant metric tensor components $g^{ij} = \nabla \xi^i \cdot \nabla \xi^j$ and the Jacobian of the transformation, $\vec{x}(\vec{\xi})$, J, as:

$$\frac{\partial}{\partial \xi^i} \left(\frac{J g^{ij}}{w} \right) = 0; {}^i j = 1,2 \qquad (1).$$

This is the (nonlinear) grid evolution equation for a given error function w (which generally depends on the solution of a physical model [4, 5]). We have succeeded in developing a scalable MG-preconditioned Newton-Krylov solver for Eq. 1, as evidenced in Table 1, where it is shown that the CPU time scales linearly (optimally) with the number of mesh points. This development opens the possibility of a simultaneous solution of the grid and physics equations in a given implicit time step. A sample 2D grid obtained with Eq. 1 for a Gaussian annulus ,

$$w = 1 + 9 * \exp[\left(r^2 - r_0^2 \right) / \sigma^2] \text{with } r_0 =$$

0.4, σ = 0.1, and r centered at $x = y = 0.5$ is shown in Fig. 1 (right).

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Figure 1—
Left and middle: efficacy plot comparing adaptive vs uniform grid solutions for heat equation (left) and Burgers equation (middle). Right: sample 2D grid for the Gaussian annulus error function.

Grid	Newton its.	Total GMRES its.	CPU(s)
32x32	7	1	10
64x64	7	3	46
128x128	7	2	170

Table 1—
Grid convergence study of Eq. 1 for the Gaussian annulus error function.